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Modeling the Process-Microstructure-Mechanical Properties in Laser Powder Bed Fusion: Review of Data-Driven Approaches and Machine Learning Strategy for Ti-6Al-4V.

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***Abstract*—**This paper reviews the modeling of the Process-Microstructure-Mechanical property in the laser powder bed fusion, focusing on the data-driven approaches, from which a strategy modeling by machine learning algorithms is established for the Ti-6Al-4V. A sensitivity and uncertainty analysis strategy is studied considering the variation of the process parameters to the microstructure features and the mechanical properties. An deep neural network (DNN) is introduced to construct a surrogate model between input parameters and microstructure features. The proposed strategy aims to deliver an efficient and cost-effective prediction of both Microstructure features and the mechanical properties of the laser powder bed fusion Ti-6al-4v. The proposed methodology achieves high predictive accuracy, as evidenced by strong correlations between predicted and actual values. Additionally, it identifies critical process parameters, such as the length of the melt pool tail, that play a significant role in determining the size of microstructure. This research provides a cost-effective approach for enhancing process optimization and quality control within the realm of metal additive manufacturing.

***Keywords-component*—Laser Powdeer Bed Fusion, Microstructure, Machine learning.**

I. INTRODUCTION

Additive manufacturing (AM) is a process of building parts layer by layer, allowing for the creation of complex geometries with reduced time and material waste. While this method offers a unique approach to the manufacturing industry, it also involves complicated processes and physics. AM technologies encompass various processes, including material technology, thermal processing, electronic systems, mechanical processes, and computer technologies.

Given this complexity, several factors—such as process parameters, material properties, and the working environment—can significantly impact the final built part, including its properties, strength, and overall quality. A fundamental question in AM is how to develop multiple performance characteristics of built parts by considering various process parameters, microstructural features, and their mechanical properties. Therefore, it is crucial to establish a process-structure-property (P-S-P) relationship to fully understand AM optimization and quality control [4].

Traditionally, the P-S-P relationship is developed through the generation of representative volume elements (RVEs) and finite element-based numerical simulations using microstructure-based models. While this approach has proven effective, it has limitations: the best structures can only be identified within a given dataset. As a result, a large dataset of microstructures is necessary to enhance the likelihood of discovering superior materials and performance outcomes [2].

In the recent years, the data-driven surrogate modelling using deep learning approaches has provided an alternative way with minimum computation cost compared to traditional ways and can combine to experimental and numerical modes to generate new data sets that would to lead to provide more accurate predictions about the microstructure and the performance. The deep learning technique has been adopted to wide fields in AM like image segmentation, microstructure generation, microstructure reconstruction and classification. The data driven predictive models provides an automatic exploration of the pattern or the trends in the data and thus help in construction of the p-s-p relationships in the parametric space and can predict on the unseen data points without the actual requirement of physic-based modelling or the experiments [3].

The present study proposes a framework for a non-intrusive deep neural network for the parametric analysis of microstructure generation in SLM-built part. This data-driven framework employs DNN model to perform the uncertainty and sensitivity

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analysis of microstructure data obtained through finite element numerical solutions. The solution matrix indicates the chord lengths of the grains present in the microstructure. This study utilizes an open-source dataset comprising 960 unique 3D microstructures, which were generated through the simulation of powder bed fusion in metal additive manufacturing (AM) provided by [4]. The data was produced using a stochastic parallel particle kinetic simulator (SPPARKS), which is based on the kinetic Monte Carlo (kMC) method and is designed to provide insights into AM microstructures.

II. Review of literature

Laser Powder Bed Fusion (LPBF) is an advanced additive manufacturing (AM) technique that enables the fabrication of intricate metal components by selectively melting thin layers of metal powder using a high-energy laser[1]. The LPBF process follows a layer-by-layer approach, where a laser scans across a pre-deposited powder bed according to a digital design, melting and solidifying the material to form a dense structure. This process is particularly suited for the Ti-6Al-4V alloy, widely used in aerospace, biomedical, and automotive applications due to its high strength, lightweight nature, and excellent corrosion resistance[2]. Studies have shown that process parameters such as laser power, scan speed, hatch spacing, and layer thickness significantly impact the thermal history and resulting microstructure of LPBF-manufactured Ti-6Al-4V.

In the production cycles of metal additive manufacturing (AM),process parameters play a crucial role in optimizing the final product [6]. Techniques such as heat treatment and machining are often implemented to refine material properties, achieve precise tolerances, and enhance surface finishes. These steps are essential because the unique and often heterogeneous microstructure characteristic of metal AM parts influences their mechanical properties in significant ways, which in turn affects their machinability.

Understanding this interplay between process parameters and microstructure is vital for optimizing performance during machining operations. Key microstructural factors—including grain morphology, which encompasses aspects such as grain size, density, orientation, residual stress, and phase fraction—can dramatically influence how these materials behave. For instance, variations in grain structure could lead to differences in mechanical performance.

Uncertainty quantification (UQ) and sensitivity analysis play a crucial role in addressing the challenges associated with product variations in manufacturing processes. By constructing models that represent product variations as functions of various contributing factors, these methodologies enable effective management of uncertainty (UM) [5]. In particular, model-based uncertainty quantification has emerged as a cost-effective and efficient strategy for ensuring quality control in production environments, largely due to advancements in simulation techniques.

While the potential benefits of model-based UQ are significant, the application of these methods within the additive manufacturing (AM) process remains in its developmental infancy. Current efforts in model-based UQ in AM are still evolving, and there is a pressing need for further research and refinement. Continued progress in this area could enhance our ability to predict outcomes, optimize processes, and ultimately improve the reliability and quality of products produced through additive manufacturing techniques.

Kamath [1] conducted a thorough investigation into the variability of the melt pool depth that arises from uncertain laser parameters. This research highlights how fluctuations in laser settings can impact the performance and outcomes of additive manufacturing processes. Similarly, Lopez et al. [8] examined the geometric variations of the melt pool, focusing on how uncertainties in both laser parameters and material properties contribute to these discrepancies. In a more recent study, Haines et al. [7] uncovered the sensitivity of a material's microstructure to its alloy composition, emphasizing the intricate relationship between grain evolution and solidification processes at a microscopic level.

Luan et al. [11] developed single crystal microstructures by implementing the Potts Monte Carlo Simulation (MCS) method. In their research, they carefully examined how their specific sampling strategy influenced the computations of several critical microstructural parameters. These parameters included not only the grain size but also the distribution of grain face numbers, which are essential for understanding the overall properties of the material. Huyse and Maes [12] focused on how uncertainties within the microstructural characteristics propagate to affect homogenized material parameters. They conducted their study by analyzing different window sizes of the actual microstructure, which allowed them to capture a range of variability in their calculations. Additionally, they utilized the MCS technique to illustrate the inherent stochastic nature of key mechanical properties, specifically Young's modulus and Poisson's ratio, thereby providing insights into how microstructural variations can lead to unpredictable changes in material behavior.

Kouchmeshky and Zabaras [13] employed a collocation approach to quantify the uncertainties in deformation responses that arise from variations in the initial microstructure induced during processing. Their work aimed to identify the extent to which these processing-induced variations can influence the mechanical performance of materials, thereby contributing to a better understanding of material reliability and consistency in engineering applications. The numerical methods for uncertatnity quantification in microstructure analysis are computationally expensive.

The field of machine learning (ML) has emerged as a significant and increasingly visible force in the realm of materials science. Researchers are drawn to ML techniques in material design because traditional experimental procedures and computational methods can often be labor-intensive, costly, and highly dependent on numerous variables that require extensive testing.

Recent studies demonstrate the versatility of ML applications across various areas within materials research. For in-

stance, ML has been effectively utilized in the design of polycrystalline materials, enabling a deeper understanding of their properties and behaviors. Additionally, it has played a crucial role in material discovery, helping to identify new compounds and materials with desirable characteristics. Another notable application involves the design of microstructures aimed at achieving specific design parameters, which is fundamental in tailoring materials for specific uses.

Furthermore, the capabilities of ML have been extended to the design and analysis of composite materials, offering innovative approaches to enhance their performance. In situations where uncertainty is a factor in material design, ML has emerged as a particularly promising tool. For example, a study by Xiao et al. [14] explored the use of ML to quantify the uncertainties arising from atomic energy surfaces, specifically in the context of titanium dioxide (TiO2), using advanced atomistic simulations.

Another investigation by Mukhopadhyay et al. [15] focused on assessing the impacts of material and structural uncertainties on the performance of functionally graded material shells. They employed a nonintrusive ML approach, highlighting the adaptability of ML in addressing complex material behavior under varying conditions.

Recently, Acar [16] contributed to the field by developing a crystal plasticity model for the Ti–7Al alloy employing supervised learning techniques. This model represents a significant advancement in the understanding and prediction of material behavior, illustrating the potential of ML to revolutionize material design and analysis in the coming years.

Although machine learning (ML) has been widely applied in additive manufacturing, there is still a significant gap in the literature regarding a systematic approach to uncertainty quantification (UQ) and uncertainty modeling (UM) throughout the various stages of the additive manufacturing process using machine learning models. Specifically, comprehensive studies are needed to link process parameters, microstructure formation, and the uncertainties that arise during the process, which ultimately affect the quality of the final product. This multilevel perspective is essential for advancing our understanding of how to optimize outcomes in additive manufacturing.

III. Machine learning Data-driven modeling strategy for Ti-6Al-4V

A. Machine learning approaches

Recent advancements in machine learning (ML) and deep neural networks (DNNs) offer a powerful approach to predicting and qualifying the microstructure of LPBF-processed Ti-6Al-4V based on process parameters. Traditional experimental and computational approaches, such as phase-field modeling and finite element simulations, are computationally expensive and time-intensive. In contrast, neural networks provide a data-driven alternative that can efficiently learn complex relationships between LPBF parameters and resulting microstructural features.

This study aims to develop a neural network-based framework for predicting and qualifying the microstructure of Ti-6Al-4V fabricated using LPBF. The proposed model leverages a dataset of process parameters and corresponding microstructural characteristics to establish predictive relationships, enabling improved process control and optimization. By integrating deep learning with experimental data, this research contributes to advancing microstructure engineering, quality assurance, and in-situ process monitoring in metal additive manufacturing.

Deep neural network: When selecting a surrogate model, multiple factors must be considered, including the specific problem, available data, computational resources, and the trade-off between performance and interpretability. Deep Neural Networks (DNNs) have become increasingly popular because of their advantages in representation learning, nonlinear modeling, scalability, end-to-end learning, and transfer learning.

In contemporary research, deep neural networks are widely employed as an effective numerical strategy for the nonlinear mapping of features (inputs) to their corresponding targets or labels (outputs). DNNs are structured with nodes; each node collects inputs, sums the associated weights, and applies activation functions to produce outputs. These nodes are organized into several layers, with nodes in one layer connected to those in the subsequent layer, while nodes within the same layer are not directly interconnected.

Deep neural networks employ parameterized functions as their basis, with the parameters being tuned throughout the training process. Additionally, the model displays nonlinearity owing to the use of nonlinear activation functions.

Figure 1 illustrates a deep neural network (DNN) consisting of one hidden layer. In this configuration, the input data is effectively transmitted to the first hidden layer (1), where it undergoes evaluation and processing.

$$H_l^{(1)} = F(\sum_{i=1}^{n} W_{li}^{(1)} x_i + a_l^{(1)}) \tag{1}$$

The inputs are then sent to the output layer, where the responses are calculated as follows:

$$y_m = G(\sum_{l=1} W_{ml}^{(0)} H_l^{(1)} + a_m^{(0)}) \tag{2}$$

F and G are the activation functions, while $W_{li}^{(1)}$ and $W_{ml}^{(0)}$ denote the weight parameters. The bias parameters are represented by $a_l^{(1)}$ and $a_m^{(0)}$. The dataset is represented as $X_D = (x_D^{(1)}, x_D^{(2)}, ..., x_D^{(N)})^T$, comprising N input vectors, with corresponding target values $Y_D = (y_D^{(1)}, y_D^{(2)}, ..., y_D^{(N)})^T$ defined by the relationship $y_D^{(i)} = M(x_D^{(i)})$. To optimize the model, we aim to minimize the error function, specifically employing the mean square error (MSE) as our loss function, which quantifies the difference between the predicted outputs and the actual labels, as formalized in Eq. 2. Additionally, to mitigate the risk of overfitting, a regularization term λ is incorporated into the error function, as detailed in Eq. 4.

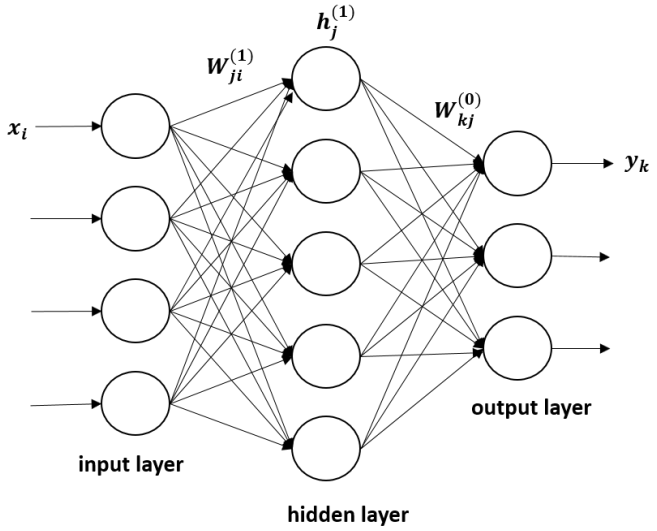

Figure. 1. A neural network with one hidden layer

$$E_D = \frac{1}{N}\sum_{i=1}^{N}\left\{\frac{1}{2}\sum_{m=1}^{n}\left[y_k^{(i)} - y_{D,k}^{(i)}\right]^2\right\} = \frac{1}{2N}\sum_{i=1}^{N}(Y_D - Y_{NN})^2 \tag{3}$$

$$J = E_D + \lambda\sum_{l,\alpha,\beta}(W_{\alpha\beta}^{(l)})^2 \tag{4}$$

An iterative approach using the backpropagation algorithm aims to minimize the error function J. Typically, the rectified linear unit serves as the activation function; however, in this regression context, G functions as an identity mapping. In Fig.2, a deep neural network is illustrated, consisting of four hidden layers, with the input layer having a dimension of $n = 6$ and the output layer having a dimension of $m = 120$. Several publicly available frameworks facilitate the implementation of standard deep neural networks, including TensorFlow, PyTorch, and Keras.

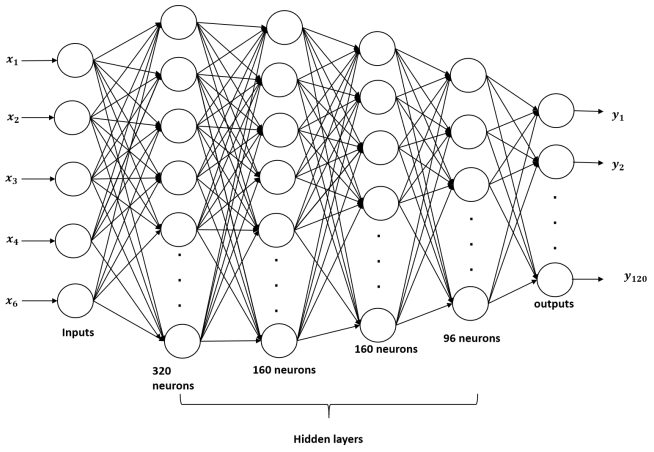

Figure. 2. A four-layer Deep neural network

B. Senstivity Analysis

Sensitivity analysis is a method used to assess how variations in input parameters affect the outputs of a model. If a small change in an input parameter leads to a relatively significant change in the output, that parameter is considered important for the model. In global sensitivity analysis, all inputs are varied simultaneously across their ranges and are typically treated as independent.

The main steps involved in global sensitivity analysis are: 1. Specifying the computational model. 2. Identifying the relevant inputs and their bounds. 3. Generating input samples using a sampling design method. 4. Evaluate the results based on the input parameters generated. 5. Conduct an uncertainty analysis and calculate the relative importance of each input using a sensitivity estimator.

For more mathematical details, refer to [4] and related references. The code described in is also applied in this case study.

IV. Results and disscusion

The objective of this study was to predict the chord length in pixels, a critical measurement in image-based process monitoring, using a set of process parameters (rotation angle per layer, melt pool characteristics, heat-affected-zone width, and velocity) as input. The DNN model was designed to capture the non-linear relationships between these inputs and the chord length, thereby providing a reliable predictive tool for process optimization. A Deep Neural Network (DNN) model was established utilizing a dataset consisting of 960 input vectors along with their corresponding chord lengths, measured in pixels, in the x, y, and z coordinates. The dataset was partitioned into training, validation, and testing subsets to facilitate the evaluation process. The optimal validation performance of the DNN model is depicted in Fig. 3, illustrating the convergence of the error function throughout the training iterations (epochs). The training curves reflect a successful learning process, with the highest validation performance achieved at epoch 204, resulting in a mean squared error (MSE) of 0.00036529. The close alignment of the training, validation, and testing curves signifies minimal overfitting and strong generalization, indicating that the finalized model is accurate and trustworthy for the specified prediction task. To evaluate the performance of our DNN model, we compared the actual chord length measurements (in pixels) with the values predicted by DNN. Figure 4 illustrates a scatter plot where: The x-axis represents the actual chord length values. The y-axis represents the predicted chord length values. The diagonal line ($y = 0.82x + 0.01$) represents perfect predictions. Ideally, all data points should lie exactly on this diagonal line, which would indicate that the predicted values match the actual measurements without any error. In our graph, most data points cluster tightly around the diagonal line, demonstrating that the model successfully captures the underlying relationship between the process parameters and the chord length in pixels.

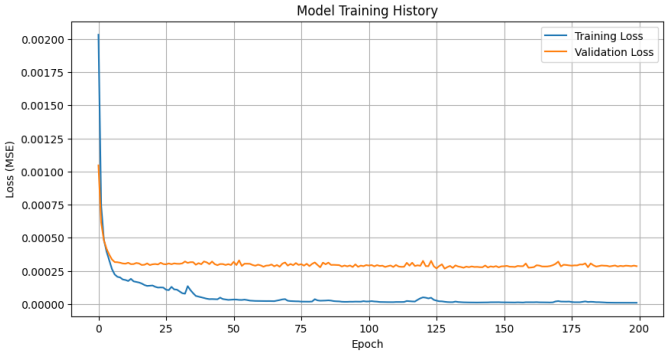

Figure. 3. Performance of DNN

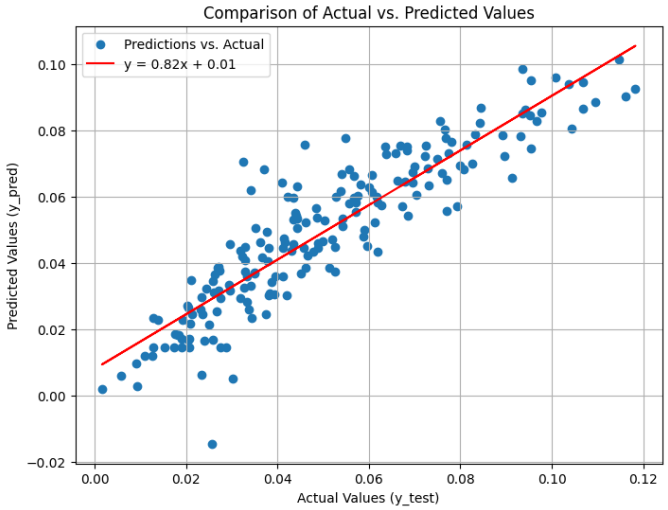

Figure. 4. Predictions for data set

Deviations are noted at both high and low chord lengths, suggesting that the model tends to either overestimate or underestimate values in these extreme regions. These discrepancies may arise from factors such as a limitation in the training data available for extreme values. An increase in measurement noise or variability in process parameters in these ranges. Overall, the close alignment of the majority of points with the diagonal line, along with a high R^2 value (closer to 1), confirms that the DNN model performs robustly in predicting chord lengths from the given process parameters. The line graph presented in Figure 5 illustrates that the predictions made by the deep neural network align closely with the actual measurements of chord length, exhibiting only minor localized discrepancies. This strong correlation signifies robust model performance and implies that, with additional refinements, the model can be reliably employed to estimate chord lengths in pixels for process monitoring and other pertinent applications.

To build the confidence on the database, a convergence study has been performed for the standard deviation with respect to different sample sizes NZ. The Sobol sampling technique (Joe and Kuo, 2008) has been used to generate the samples by varying the size NZ from small values to a relatively

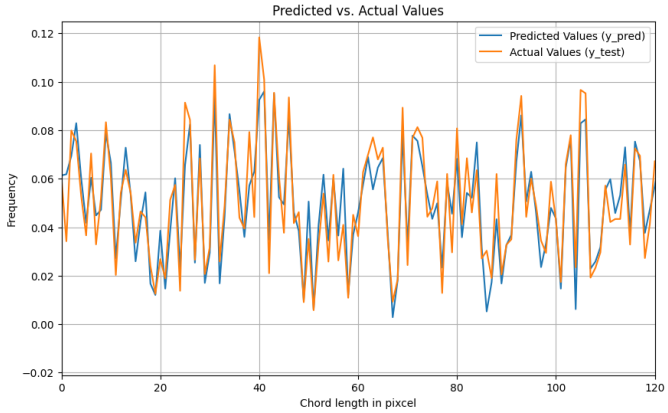

Figure. 5. Scatter plot of Actual vs. Predicted Chord Lengths

large values (NZ= 600, 900, 2000, 5000, ... upto 35000). The corresponding outputs (chord length) are predicted through DNN model. To check the convergence for this statistical study, plots for the standard deviation with respect to the sample size is shown Figure 6 . The standard deviations show some fluctuations by increasing the sample size up to 10000; however, between sample sizes 10000 to 35000, the standard deviation is close to a constant (up to 1% of variation) which implies that the sample size 10000 is reasonably sufficient for the oncoming sensitivities and uncertainity analyses.

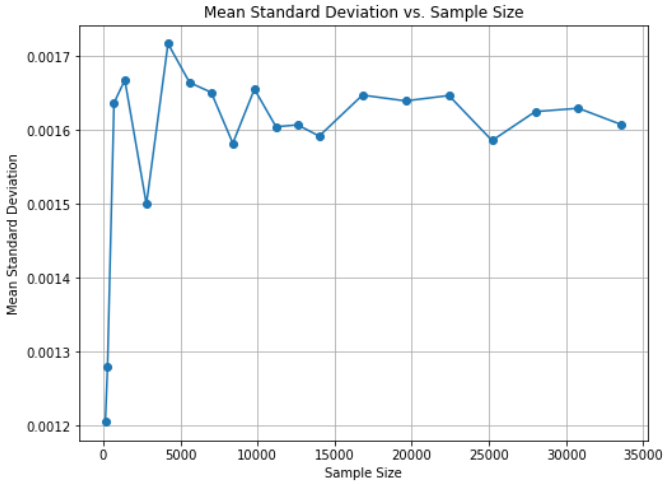

Figure. 6. Convergence study of samples

Using the obtained standard deviations, confidence intervals for the numerical vertical results (mean +- 2 standard deviation) are represented in Figure 7. The chord length in pixels along frequencies are represented on this figure. The initial 40 chord lengths are aligned along the x-axis, the subsequent 40 lengths extend along the y-axis, and the final 40 lengths pertain to the z-axis. In all coordinates, initially the data show some fluctuations, however, the behaviour is very smooth. Figure 7 shows that the length of the chord in pixels, when considering their uncertainties, is mainly within

the predicted confidence intervals, the numerical confidence intervals could be 'enlarged' by changing the probability distributions of the input parameters. Indeed, we have used prior uniform distributions on estimated input intervals (using expert judgment).

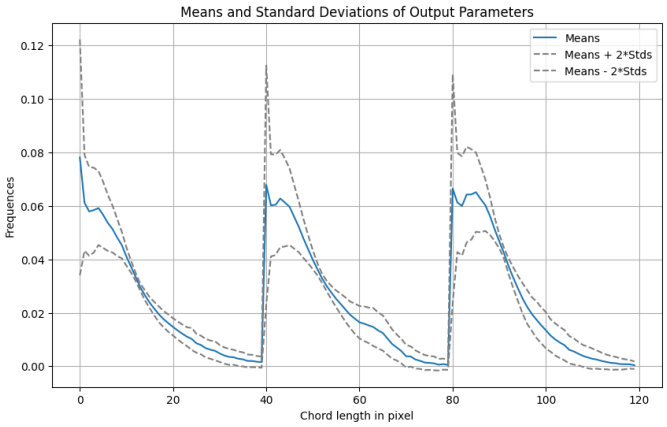

Figure. 7. Uncertainity analysis

The Sobol indices are defined as the ratio of partial variances to the total variance, which reflect the relative importance of each input parameter as shown in Figure 8. It is clear in the Figure 8 that the Meltpool tail length is the dominant parameter with a contribution of 55%, Rotation angle is the second most significant parameter, with less effect (23%).

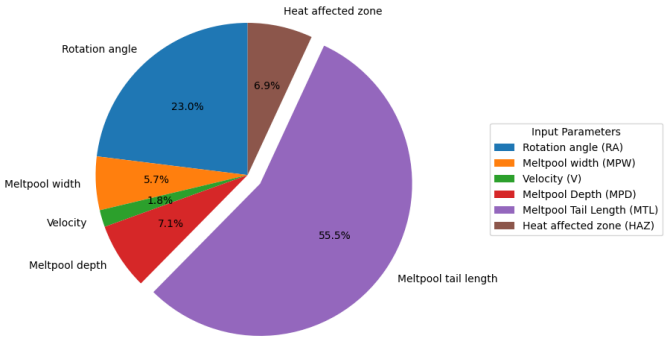

Figure. 8. Senstivity analysis of parameters

V. Conclusion

This study introduces a comprehensive, data-driven framework for modeling the complex relationships among process parameters, microstructural evolution, and mechanical performance in titanium alloy Ti-6Al-4V produced through laser powder bed fusion (LPBF). By integrating deep neural networks with rigorous sensitivity and uncertainty analyses, the proposed model effectively predicts key microstructural characteristics, such as chord lengths, and establishes correlations with the corresponding mechanical properties. The findings emphasize the critical influence of process parameters, particularly the melt pool tail length and rotation angle, on material behavior. Convergence studies and confidence interval analyses further validate the model's robustness, demonstrating its potential as a valuable tool for process monitoring and optimization. Future research will aim to expand the dataset, investigate additional alloy systems, and refine the model to enhance its capacity to accurately represent extreme processing conditions, thus advancing the development of more reliable and scalable additive manufacturing solutions.

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